Metastability and Dominant Eigenvalues of Transfer Operators

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Abstract

We prove upper and lower bounds for the metastability of a state-space decomposition for reversible Markov processes in terms of dominant eigenvalues and eigenvectors of the corresponding transfer operator. The bounds are explicitly computable and sharp. In contrast to many other approaches, the results do not rely on any asymptotic expansions in terms of some smallness parameter, but rather hold for arbitrary transfer operators satisfying a reasonable spectral condition.

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1 Introduction

There are many problems in physics, chemistry or biology where the length and time scales corresponding to the microscopic descriptions (given in terms of some stochastic or deterministic dynamical system), and the resulting macroscopic effects differ many orders of magnitude. Rather than resolving all microscopic details, often one is interested in characteristic features on a macroscopic level (e.g., phase transitions, conformational changes of molecules, climate changes etc.). A typical mathematical example is the

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limit behavior for "time to infinity", where invariant measures or limit cycles are established characteristic objects (e.g., [22, 24]). Metastability is another important characteristics which is related to the long time behavior of the dynamical system. It refers to the property that the dynamics is likely to remain within a certain part of the state space for a long period of time, until it eventually exits and transits to some other part of the state space. There are well-established links of metastability to, e.g., exit times [3, 14, 15], eigenvalues of transfer operators or generators [3, 10, 9, 7, 27], phase transitions [2, 6], reduced Markovian approximations [27, 20, 21], averaging [28], and many other areas.

There is no unique but several characterizations of metastability in the literature (see, e.g., [2, 7, 27, 30]). There are at least two different conceptual approaches to metastability. (1) A subset C is called metastable, if the fraction of systems in C (measured w.r.t. some pre-specified probability measure), whose trajectory exits during some pre-defined microscopic time span, is significantly small. (2) A subset C is called metastable, if with high probability a typical long–term trajectory stays within C longer than some macroscopic time span. Thus, in broad terms, you may either observe an ensemble of systems for a short time or a typical system for a long time to characterize metastability. We will restrict our attention to the ensemble approach, the use of which was motivated by a molecular application (conformation dynamics, see [11, 26, 27]), where the probability measure is given by the canonical ensemble or Boltzmann distribution, while the observation time span is linked to the experimental setting.

We will assume that the dynamical system is given in terms of some reversible Markov chain with invariant measure μ. Equivalently, we may specify the dynamics in terms of the associated transfer operator P acting on $L^2(\mu)$ and being self-adjoint due to reversibility. There is a classical connection between invariant (stable) subsets and degeneracy of the maximal eigenvalue 1 of P. The degeneracy of 1 is just the number of invariant subsets of the state space (see e.g. [13, 19].) Analogously, to each eigenvalue close to 1 there corresponds an almost invariant or metastable subset of the state space, see e.g. [8, 9, 10].

Pursuing along this analogy, there is a large amount of literature relating metastability and eigenvalues of transfer operators or generators corresponding to the underlying Markov process. However, the theoretical investigations are either restricted to the finite dimensional state space case (and thus related to stochastic matrices or Laplace matrices), e.g., [17, 16, 18, 23, 29], or stated asymptotically in terms of some smallness parameter, e.g., [14]. General state space non-asymptotic results are much more rare and may be found in the setting of exit times [4, 5] or in the setting of symmetric Markov semigroups [7, 8, 30]. To our knowledge, for the general state space case in the ensemble characterization of metastability, there are no lower bounds on the metastability of an finite number of subsets in terms of eigenvalues known. It is our aim to derive an upper and in particular a lower bound on the metastability of an arbitrary decomposition from spectral properties of the transfer operator P. Such bounds are not only of theoretical interest, but also of algorithmic relevance, e.g., in the context of dynamical clustering [10, 12].

The paper is organized as follows: In Section 1.1, we introduce the set-up including the definition of metastability and its transfer operator formulation. In Section 2, a variational formula for the Rayleigh-trace of self-adjoint operators is reviewed, which is crucial in the proofs of our results. We prove upper and lower bounds for the metastability under some quite general spectral assumption on P. In Section 3, we restrict our attention to strongly continuous semigroups and prove the existence of metastable decompositions based on the spectral structure of the associated generator. Finally, in Section 4 we state some examples illustrating the sharpness and usefulness of the bounds.

1.1 Markov chains, transfer operators and metastability

Throughout let $X = (X_n)_{n\in\mathbb{N}}$ denote a homogeneous Markov chain on the state space $\mathcal{X}$ with transition kernel

$$p(x, A) \quad = \quad \mathbb{P}[X_1 \in A | X_0 = x], \tag{1}$$

for all $x \in \mathcal{X}$ and all subsets $A \subset \mathcal{X}$ contained in the σ–algebra $\mathcal{A}$. Consider a probability measure μ on $\mathcal{X}$ and assume that the Markov chain is initially distributed according to ν, i.e., $X_0 \sim \nu$ meaning

$$\mathbb{P}[X_0 \in A] \quad = \quad \nu(A) \tag{2}$$

for all $A \in \mathcal{A}$. Then, the Markov chain at time $k > 0$ is distributed according to

$$\mathbb{P}[X_k \in A | X_0 \sim \nu] \quad = \quad \mathbb{P}_\nu[X_k \in A] \;=:\; \nu_k(A).$$

The time-evolution of probability measures $\{\nu_k\}$ can be described by the transfer operator P acting on the space of bounded measures on $(\mathcal{X}, \mathcal{A})$ via

$$P\nu(A) \quad = \quad \mathbb{P}_\nu[X_1 \in A] = \int_{\mathcal{X}} p(x, A)\nu(dx). \tag{3}$$

Assume that the Markov chain exhibits a unique invariant probability measure μ, i.e., $P\mu = \mu$ and define the weighted Hilbert space of measurable functions

$$L^2(\mu) \quad = \quad \{f : \mathcal{X} \to \mathbb{R} : ||f||^2 \int_{\mathcal{X}} |f(x)|^2 \mu(dx) < \infty\}.$$

with inner product given by

$$\langle f, g \rangle \quad = \quad \int_{\mathcal{X}} f(x) g(x) \mu(dx).$$

If μ is the invariant probability measure of P, then $\nu_0 \ll \mu$ implies $\nu_t \ll \mu$ [25, Chapter 4]. Hence we may consider P as an operator on $L^m(\mu)$ acting on probability measures that are absolutely continuous w.r.t. μ according to

$$\int_A Pv(x)\mu(dx) \quad = \quad \int_{\mathcal{X}} p(x, A) v(x) \mu(dx).$$

In the sequel we assume that the Markov chain X is reversible, hence the transition kernel satisfies

$$\mu(dx) p(x, dy) \quad = \quad \mu(dy) p(y, dx).$$

As a consequence, P is self-adjoint on $L^2(\mu)$.

We now introducing the notion of the transition probabilities between subsets (see [27, 19]), in terms of which metastability will be defined:

Definition 1.1 *Let $A, B \subset \mathcal{X}$ denote measurable subsets of the state space.*

(i) The transition probability from A to B is defined to be the conditional probability

$$p(A, B) \quad = \quad \mathbb{P}_\mu[X_1 \in B | X_0 \in A] \; = \; \frac{1}{\mu(A)} \int_A p(x, B) \mu(dx),$$

if $\mu(A) > 0$ and $p(A, B) = 0$ otherwise. In other words, the transition probability quantifies the dynamical fluctuations within the invariant distribution μ.

(ii) A subset $A \in \mathcal{A}$ is called invariant, if $p(A, A) = 1$.

(iii) A subset $A \in \mathcal{A}$ is called metastable, if $p(A, A) \approx 1$. Hence, metastability is almost invariance.

Requiring the transition probability to be "close to 1" is obviously a vague statement—however, in most applications we are interested in a decomposition into the most metastable subsets, which eliminates the problem of interpreting "close to 1". Instead we have to determine the number of subsets, we are looking for. This is done by examining the spectrum of the transfer operator P. Alternatively, we could determine a cascade of decompositions with an increasing number of metastable subsets.

It is easy to see that the transition probability between subsets can be rewritten in terms of the inner product $\langle \cdot, \cdot \rangle$ according to

$$p(A, B) = \frac{\langle P\mathbf{1}_A, \mathbf{1}_B \rangle}{\langle \mathbf{1}_A, \mathbf{1}_A \rangle}, \tag{4}$$

where $\mathbf{1}_A$ denotes the characteristic function of the subset A.

Consider a decomposition of the state space $\mathcal{X}$ into mutually disjoint subsets $\mathcal{D} = \{A_1, \ldots, A_n\}$. Then,

$$m(\mathcal{D}) = p(A_1, A_1) + \ldots + p(A_n, A_n)$$

can be thought of as a measure of metastability of the decomposition $\mathcal{D}$. It is our aim to get upper and lower bounds on the metastability of the decomposition in terms of eigenvalues and corresponding eigenvectors of the transfer operator.

We are interested in situations, where the spectrum of the transfer operator satisfies the following

> **Assumption S:** The transfer operator $P : L^2(\mu) \to L^2(\mu)$ is self–adjoint and exhibits n eigenvalues
>
> $$\lambda_n \leq \ldots \leq \lambda_2 < \lambda_1 = 1,$$
>
> counted according to their multiplicity. The corresponding set of μ–orthonormal eigenvectors will be denoted by $\{v_n, \ldots, v_1\}$. Furthermore, the spectrum $\sigma(P)$ of P satisfies
>
> $$\sigma(P) \subset [a, b] \cup \{\lambda_n, \ldots, \lambda_2, 1\}$$
>
> for some constants $a, b \in (-1, +1)$ satisfying $-1 < a \leq b < \lambda_n$. In this sense, the eigenvalues are called dominant.

In particular, the Assumption S is satisfied, if the underlying Markov chain is reversible and geometrically or V-uniformly ergodic (see, e.g., [19, Thm. 4.31]), which is always the case, if the state space is finite dimensional (and the Markov chain reversible).

2 Upper and Lower Bounds

This section proves upper and lower bounds on the metastability of an arbitrary decomposition of the state space in terms of dominant eigenvalues and eigenvectors of the transfer operator corresponding to the dynamics of the Markov process.

Recall that by Rayleigh's Principle the kth largest eigenvalue λ_k for $1 \le k \le n$, is given by the variational formula

$$\lambda_k \quad = \quad \max\{\langle Pw, w\rangle : w \in L^2(\mu), \|w\|_2 = 1, w \perp v_1 \dots, v_{k-1}\}.$$

where $\perp$ denotes orthogonality w.r.t. the inner product $\langle\cdot,\cdot\rangle$. The above variational formula can be generalized (for our purpose) in the following way: Consider a finite dimensional subspace U of $L^2(\mu)$ with orthonormal basis $(\varphi_1, \dots, \varphi_n)$. Then, for a self-adjoint operator P on $L^2(\mu)$ the Rayleigh-trace w.r.t. U is defined as

$$\mathrm{Tr}_U P \quad = \quad \sum_{i=1}^{n} \langle P\varphi_i, \varphi_i\rangle.$$

Note that this definition is independent of the particular choice of the orthonormal basis (see, e.g., [1]).

Theorem 2.1 *Assume that $P : L^2(\mu) \to L^2(\mu)$ is a self adjoint transfer operator satisfying Assumption S on its spectrum. Then*

$$\begin{aligned}
&\lambda_n + \ldots + \lambda_1 \\
&\quad = \quad \max\{\, \mathit{Tr}_U P : U \text{ is } n\text{-dimensional subspace}\} \\
&\quad = \quad \max\left\{ \sum_{i=1}^{n} \langle P\varphi_i, \varphi_i\rangle : (\varphi_1, \ldots, \varphi_n) \text{ is orthonormal system.} \right\}
\end{aligned}$$

The above proposition is actually known to hold for every self-adjoint bounded operator P on a Hilbert space H. For convenience of the reader we give a proof, following [1]:

Proof: The second equality is clear. For $k \le n$ denote by v_k the eigenvector of P corresponding to λ_k. Setting $\varphi_i = v_i$ we easily see that

$$\lambda_1 + \ldots + \lambda_n \quad \le \quad \max\{\mathrm{Tr}_U P : U \text{ an } n\text{-dimensional subspace}\}.$$

Now let U be an arbitrary n-dimensional subspace. In order to prove $\lambda_1 + \ldots + \lambda_n \geq \mathrm{Tr}_U P$, we inductively construct orthonormal vectors $w_k \in U$, $1 \leq k \leq n$, such that $w_k \perp v_1, \ldots, v_{k-1}$. Having succeeded, we deduce from the Rayleigh principle that $\lambda_k \geq \langle P w_k, w_k \rangle$ and thus

$$\sum_{i=1}^{n} \lambda_i \geq \sum_{i=1}^{n} \langle P w_i, w_i \rangle = \mathrm{Tr}_U P.$$

To start, choose w_n to be a normalized vector $w_n \in U$ orthogonal to $\mathrm{span}\{v_1, \ldots, v_{n-1}\}$. Now if $w_n, \ldots, w_{k+1}$ have been defined, choose w_k to be a normalized vector in the k-dimensional subspace $U \cap \mathrm{span}\{w_{k+1}, \ldots, w_n\}^{\perp}$, which is perpendicular to $\mathrm{span}\{v_1, \ldots, v_{k-1}\}$. □

The generalized Rayleigh Principle can be exploited to prove upper bounds on the metastability of some (arbitrary) partition $A_1, \ldots, A_n$ of the state space $\mathcal{X}$ that satisfies $\mu(A_k) > 0$ for $k = 1, \ldots n$. Recall that the orthogonal projection $Q : L^2(\mu) \to L^2(\mu)$ onto $\mathrm{span}\{\mathbf{1}_{A_1}, \ldots, \mathbf{1}_{A_n}\}$ is defined as

$$Q\,v \;=\; \sum_{k=1}^{n} \frac{\langle v, \mathbf{1}_{A_k} \rangle}{\langle \mathbf{1}_{A_k}, \mathbf{1}_{A_k} \rangle} \mathbf{1}_{A_k} \;=\; \sum_{k=1}^{n} \langle v, \chi_{A_k} \rangle \chi_{A_k}.$$

with

$$\chi_{A_k} \;=\; \frac{\mathbf{1}_{A_k}}{\sqrt{\langle \mathbf{1}_{A_k}, \mathbf{1}_{A_k} \rangle}}$$

for $k = 1, \ldots, n$ and for every $v \in L^2(\mu)$. We are now ready to state

Corollary 2.2 *Consider some transfer operator $P : L^2(\mu) \to L^2(\mu)$ satisfying Assumption S on its spectrum. Then*

$$p(A_1, A_1) + \ldots + p(A_n, A_n) \;\leq\; \lambda_1 + \ldots + \lambda_n.$$

Proof: Since $p(A_k, A_k) = \langle P\chi_{A_k}, \chi_{A_k} \rangle$ using (4) and the definition of χ_{A_k}, we have

$$\sum_{k=1}^{n} p(A_k, A_k) \;=\; \sum_{k=1}^{n} \langle P\chi_{A_j}, \chi_{A_j} \rangle. \tag{5}$$

By proposition 2.1 the right hand side of (5) is less or equal to $\lambda_1 + \ldots + \lambda_n$, since $\{\chi_{A_1}, \ldots, \chi_{A_n})$ is an orthonormal basis of $\mathrm{span}\{\mathbf{1}_{A_1}, \ldots, \mathbf{1}_{A_n}\}$. □

We now prove the lower bound on metastability.

Proposition 2.3 *Consider some transfer operator $P : L^2(\mu) \to L^2(\mu)$ satisfying Assumption S on its spectrum. Then*

$$\rho_1\lambda_1 + \ldots + \rho_n\lambda_n + c \leq p(A_1, A_1) + \ldots + p(A_n, A_n), \tag{6}$$

where $\rho_j = \|Qv_j\|^2 = \langle Qv_j, Qv_j\rangle \in [0,1]$ and[1] *$c = a\,((1-\rho_1) + \ldots + (1-\rho_n))$. In particular, if $\{\varphi_1, \ldots, \varphi_n\}$ is an arbitrary orthonormal basis of span$\{\mathbf{1}_{A_1}, \ldots, \mathbf{1}_{A_n}\}$, then*

$$\kappa_1\lambda_1 + \ldots + \kappa_n\lambda_n + c \leq p(A_1, A_1) + \ldots + p(A_n, A_n), \tag{7}$$

where $\kappa_j = |\langle v_j, \varphi_j\rangle|^2 \in [0,1]$.

Proof: Denote by $\Pi : L^2(\mu) \to \mathrm{span}\{v_1, \ldots, v_n\}$ the orthogonal projection onto the subspace spanned by the maximal eigenvectors, and set $\Pi^\perp = \mathrm{Id} - \Pi$. Then

$$\begin{aligned}
\sum_{j=1}^n p(A_j, A_j) &= \sum_{j=1}^n \langle (P - a\mathrm{Id})\chi_{A_j}, \chi_{A_j}\rangle + \sum_{j=1}^n a\,\langle \chi_{A_j}, \chi_{A_j}\rangle \\
&= \sum_{j=1}^n \Big\langle ((P - a\mathrm{Id})\Pi + (P - a\mathrm{Id})\Pi^\perp)\chi_{A_j}, (\Pi + \Pi^\perp)\chi_{A_j}\Big\rangle \\
&\quad + an \\
&= \sum_{j=1}^n \Big\langle (P - a\mathrm{Id})\Pi\chi_{A_j}, \Pi\chi_{A_j}\Big\rangle \\
&\quad + \sum_{j=1}^n \Big\langle (P - a\mathrm{Id})\Pi^\perp\chi_{A_j}, \Pi^\perp\chi_{A_j}\Big\rangle + an.
\end{aligned}$$

The first two terms of the right hand side can be further analyzed:

$$\begin{aligned}
\sum_{j=1}^n \Big\langle (P - a\mathrm{Id})\Pi\chi_{A_j}, \Pi\chi_{A_j}\Big\rangle &= \sum_{j=1}^n \Big\langle \sum_{k=1}^n (\lambda_k - a)\langle\chi_{A_j}, v_k\rangle v_k, \sum_{l=1}^n \langle\chi_{A_j}, v_l\rangle v_l\Big\rangle \\
&= \sum_{j=1}^n \sum_{k=1}^n (\lambda_k - a)\langle\chi_{A_j}, v_k\rangle^2 \\
&= \sum_{k=1}^n (\lambda_k - a)\langle Qv_k, Qv_k\rangle.
\end{aligned}$$

[1] The constant a is defined in the Assumption S.

To proof the first statement, we remark that $\langle (P - a\mathrm{Id})\Pi^{\perp}\chi_{A_j}, \Pi^{\perp}\chi_{A_j}\rangle$ is non–negative, since $P - a\mathrm{Id}$ is non-negative definite according to the assumptions made. Hence,

$$\sum_{j=1}^{n} p(A_j, A_j) \geq \sum_{k=1}^{n} \lambda_k \rho_k + a \sum_{k=1}^{n} (1 - \rho_k).$$

For the second statement simply note that

$$\rho_j \;=\; \langle Qv_j, Qv_j\rangle \;=\; \sum_{k=1}^{n} |\langle v_j, \varphi_k\rangle|^2 \;\;\geq\;\; |\langle v_j, \varphi_j\rangle|^2 \;=\; \kappa_j,$$

which completes the proof. □

Invariance of μ implies $v_1 = \mathbf{1}_{\mathcal{X}}$ and thus $\rho_1 = \|Qv_1\|^2 = 1$. Summarizing, our central result is

Theorem 2.4 *Consider some transfer operator $P : L^2(\mu) \to L^2(\mu)$ satisfying Assumption S on its spectrum. Then the metastability of an arbitrary decomposition $\mathcal{D} = \{A_1, \ldots, A_n\}$ of the state space can be bounded from above by*

$$p(A_1, A_1) + \ldots + p(A_n, A_n) \leq 1 + \lambda_2 + \ldots + \lambda_n,$$

while it is bounded from below by

$$1 + \rho_2\lambda_2 + \ldots + \rho_n\lambda_n + c \leq p(A_1, A_1) + \ldots + p(A_n, A_n)$$

where $\rho_j = \|Qv_j\|^2 = \langle Qv_j, Qv_j\rangle \in [0, 1]$ and

$$c = a\,(n - (1 + \rho_2 + \ldots + \rho_n)).$$

In particular we have $c \geq 0$ if $\sigma(P) \subset [0, 1]$.

Proof: Clear by Corollary 2.2 and Proposition 2.3. □

Remark. Note that the central Theorem 2.4 does hold for an arbitrary transfer operator satisfying Assumption S. In particular, we did not assume any asymptotics in some smallness parameter κ in order to prove some asymptotic result for $\kappa \to 0$. This is a remarkable difference to other approaches. Moreover the lower bounds are explicitly computable given some decomposition of the state space. Hence, comparing the lower and upper bound one is able to "judge" the quality of the decomposition.

In some situations, we additionally know that P is positive. For instance, if we consider the case of $P = P_\tau$, where $(P_t)_{t\geq 0}$ is a semigroup of transfer operators and τ is some fixed time. Then, we can state:

Theorem 2.5 *Consider a reversible homogeneous continuous-time Markov process $X = (X_t)_{t\in[0,\infty)}$ and its corresponding semigroup of transfer operators $P_t : L^2(\mu) \to L^2(\mu)$. If $P = P_\tau$ satisfies Assumption S on its spectrum for some fixed $\tau > 0$, then*

$$1 + \ldots + \rho_n \lambda_n \leq p(A_1, A_1) + \ldots + p(A_n, A_n) \leq \lambda_1 + \ldots + \lambda_n, \qquad (8)$$

where λ_k denote eigenvalues of the operator P_τ.

Proof: Simply note, that $P = P_\tau$ is positive, since $P = P_{\tau/2} P_{\tau/2}$, and apply Theorem 2.4 (with $a = 0$). $\square$

3 Metastable Decompositions

Up to now we have proven upper and lower bounds for an arbitrarily given decomposition of the state space. We now indicate how to guarantee minimal metastability of the Markov process. More exactly, we use the results in Davies [8] to obtain a state space decomposition with large lower bound for its metastability in Theorem 2.5. First we briefly recall the main theorem of [8].

Suppose (e^{-Ht}) is a strongly continuous one-parameter semigroup on $L^2(\mu)$ satisfying

(H1) the generator H is a non-negative self-adjoint operator on $L^2(\mu)$;

(H2) the semigroup (e^{-Ht}) is positivity preserving;

(H3) one has $e^{-Ht}\mathbf{1} = \mathbf{1}$ for all $t \geq 0$ or, equivalently, $H\mathbf{1} = 0$;

(H4) there exists $0 < \varepsilon < 1$ such that

$$\sigma(H) \subset [0, \varepsilon] \cup [1, \infty);$$

(H5) if f lies in the spectral subspace $\mathcal{H}$ of H associated with the interval $[0, \varepsilon]$, then $\|f\|_\infty < \infty$.

In [8], Davies remarks that (H5) is often provable for differential operators by the use of elliptic regularity conditions.

Under the assumptions (H1)-(H5) it is proven that there exists $c < \infty$ such that

$$c^{-1}\|f\|_\infty \leq \|f\| \leq c\|f\|_1.$$

uniformly for all $f \in \mathcal{H}$ [8]. Define $\dim(\mathcal{H}) =: n < \infty$ and note that, as before $\|\cdot\|$ denotes the 2-norm. Then the main result is proven in ([8, Theorem 19]):

Theorem 3.1 *There exists a decomposition*

$$\mathcal{X} = A_1 \,\dot{\cup}\, \ldots \,\dot{\cup}\, A_n$$

with $\mu(A_i) \geq 1/(2c^2)$ and a basis $(f_1, \ldots, f_n)$ of $\mathcal{H}$ such that

$$\|f_i - \mathbf{1}_{A_i}\| \leq 4n^{3/2}\varepsilon^{1/2}$$

for ε sufficiently small (depending on c).

Assume we are given such an H with $\varepsilon \ll 1$ (the only interesting regime). First observe that Theorem 3.1 implies

$$\begin{aligned}
\left\|\frac{f_i}{\|f_i\|} - \chi_{A_i}\right\| &\leq \left\|\frac{f_i}{\|f_i\|} - \frac{f_i}{\|\mathbf{1}_{A_i}\|}\right\| + \left\|\frac{f_i}{\|\mathbf{1}_{A_i}\|} - \frac{\mathbf{1}_{A_i}}{\|\mathbf{1}_{A_i}\|}\right\| \\
&\leq \frac{\|f_i\|_\infty}{\|f_i\|\|\mathbf{1}_{A_i}\|}\|f_i - \mathbf{1}_{A_i}\| + \frac{\|f_i - \mathbf{1}_{A_i}\|}{\|\mathbf{1}_{A_i}\|} \\
&\leq \frac{1+c}{\|\mathbf{1}_{A_i}\|}\|f_i - \mathbf{1}_{A_i}\| \\
&\leq \sqrt{2}c(1+c) \cdot 4n^{3/2}\varepsilon^{1/2} =: \delta, \qquad (9)
\end{aligned}$$

where we exploited $\|fg\| \leq \|f\|_\infty\|g\|$ for the second inequality. Now consider $v \in \mathcal{H}$, say $v = \sum_i \alpha_i f_i/\|f_i\|$. Define w by $w = \sum_i \alpha_i \chi_{A_i}$. Then by (9)

$$\|v - w\| \;\leq\; \sum_i |\alpha_i|\delta \;\leq\; \delta n^{1/2}\left(\sum_i |\alpha_i|^2\right)^{1/2} \;=\; \delta n^{1/2}\|w\|$$

and so if $\delta n^{1/2} < 1$

$$\|w\| \leq (1 - \delta n^{1/2})^{-1} \|v\|.$$

In particular if v has norm 1 these two equations show that

$$\begin{aligned} |\|Qv\| - 1| &= |\|Qv\| - \|v\|| \leq \|Qv - v\| \\ &\leq \|Qv - Qw\| + \|w - v\| \\ &\leq 2\|w - v\| \leq 2\delta n^{1/2} \|w\| \\ &\leq \frac{2\delta n^{1/2}}{1 - \delta n^{1/2}}. \end{aligned}$$

For ε sufficiently small we thus have the following

Corollary 3.2 *Consider a reversible homogeneous continuous-time Markov process $X = (X_t)_{t \in [0,\infty)}$ whose semigroup of transfer operators $P_t = e^{-Ht}$: $L^2(\mu) \to L^2(\mu)$ is strongly continuous and satisfies (H1) – (H5). Then $P = P_\tau$ satisfies Assumption S on its spectrum for fixed $\tau > 0$ with $\lambda_n \geq e^{-\varepsilon\tau}$, $a = 0$ and $b \leq e^{-\tau}$. Then, there exists a decomposition of the state space into n mutually disjoint subsets $A_1, \ldots, A_n$ whose metastability satisfies*

$$|p(A_1, A_1) + \ldots + p(A_n, A_n) - (\lambda_1 + \ldots + \lambda_n)| \leq \frac{4C(\varepsilon)n}{1 - C(\varepsilon)}.$$

with $C(\varepsilon) = \sqrt{32}c(1+c)n^2\varepsilon^{1/2}$, c defined in Theorem 3.1, and ε sufficiently small (possibly depending on c).

Proof: The statements on the spectral properties of P are clear by $P = e^{-H\tau}$. For the estimate of the metastability we just note that by the calculations preceding Cor 3.2 and setting $v = v_j$, we get

$$\rho_j = \|Qv_j\|^2 \geq \left(1 - \frac{2\delta n^{1/2}}{1 - \delta n^{1/2}}\right)^2 \geq 1 - 2\frac{2\delta n^{1/2}}{1 - \delta n^{1/2}},$$

which directly implies the assertion by inserting δ according to eq. (9). □

Remark. Davies [8] notes that it seems plausible that one could weaken the condition "ε sufficiently small (possibly depending on c)" by requiring that $0 < \varepsilon < n'$ where n' depends upon n alone. For the case $n = 2$ this is proven [7, 8].

Under additional conditions, the above result can be extended to prove asymptotic exactness of the upper and lower bounds on metastable decompositions.

Corollary 3.3 *Consider an ε-depending family of reversible homogeneous continuous-time Markov process $X_\varepsilon = (X_{\varepsilon,t})_{t\in[0,\infty)}$ whose semigroup of transfer operators $P_{\varepsilon,t} = e^{-H_\varepsilon t} : L^2(\mu) \to L^2(\mu)$ is strongly continuous and satisfies (H1) – (H5). Moreover, assume that*

(E1) there exists $n \in \mathbb{N}$ such that the dimension of the spectral subspace $\mathcal{H}_\varepsilon$ associated with the interval $[0,\varepsilon]$ satisfies $\dim(\mathcal{H}_\varepsilon) = n$ for all $\varepsilon > 0$, and

(E2) there exists $c < \infty$ such that

$$c^{-1}\|f_\varepsilon\|_\infty \le \|f_\varepsilon\| \le c\|f_\varepsilon\|_1$$

for all $f_\varepsilon \in \mathcal{H}_\varepsilon$ and all $\varepsilon > 0$.

Then, there exists a decomposition of the state space into n mutually disjoint subsets $A_{\varepsilon,1}, \ldots, A_{\varepsilon,n}$, and $C > 0$ independent of ε such that

$$n\exp(-\tau\varepsilon)\left(1 - C\varepsilon^{1/2}\right) \le p(A_{\varepsilon,1}, A_{\varepsilon,1}) + \ldots + p(A_{\varepsilon,n}, A_{\varepsilon,n}) \le n.$$

Note that $\exp(-\tau\varepsilon)(1 - C\varepsilon^{1/2}) \to 1$ as $\varepsilon \to 0$.

4 Illustrative Examples

The following example proves that both, the lower and the upper bound are sharp. Moreover the bounds are asymptotically exact in the sense that when metastability increases to invariance—and hence the metastability of the decomposition tends to n, the number of subsets of the decomposition—, then each of the dominant eigenvalues approximates 1, implying convergence of the upper bound to n, while the corresponding dominant eigenfunctions, under appropriate continuity assumptions, get more and more constant on the subsets of the decomposition, implying convergence of the lower bound to n, too.

Example 4.1 *Let $\mathcal{X} = \{0,1,2\}$ and the transition probability P be given by*

$$P = \begin{pmatrix} 0.90 & 0.05 & 0.05 \\ 0.05 & 0.05 & 0.90 \\ 0.05 & 0.90 & 0.05 \end{pmatrix}.$$

Clearly P is ergodic, and since it is symmetric the measure μ given by $\mu(\{0\}) = \mu(\{1\}) = \mu(\{2\}) = 1/3$ is invariant. The eigenvalues λ_j and corresponding eigenvectors v_j are calculated to be

$$\lambda_1 = 1, \quad \lambda_2 = 0.85, \quad \lambda_3 = -0.85$$

and (we do not need v_3)

$$v_1 = \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}, \quad v_2 = \frac{1}{\sqrt{2}} \begin{pmatrix} 2 \\ -1 \\ -1 \end{pmatrix}.$$

Consider the partition $(A_1, A_2) = (\{0,1\}, \{2\})$. The resulting metastability is given by $p(A_1, A_1) + p(A_2, A_2) = 0.525 + 0.05 = 0.575$, which is bounded from above by $1 + \lambda_2 = 1.85$. Calculating the lower bound from Theorem 2.4, we obtain (here the correction term is $c = -0.6375$)

$$0.575 = 1 + \rho_2\lambda_2 + c \leq p(A_1, A_1) + p(A_2, A_2) = 0.575,$$

which furthermore proves that the lower bound is sharp.

Now consider the partition $(A_1, A_2) = (\{0\}, \{1,2\})$. The resulting metastability is given by

$$p(A_1, A_1) + p(A_2, A_2) = 0.90 + 0.95 = 1.85,$$

which in this case is equal to the upper and lower bound

$$1 + \lambda_2 = 1.85 \text{ and } 1 + \rho_2\lambda_2 + c = 1.85,$$

since $\rho_1 = \rho_2 = 1$ and $c = 0$. This additionally proves that the upper bound is sharp, too. Note that although $\lambda_3 = -0.85$ is large negative, the correction term c does not necessarily result in some lower bound that underestimates the metastability of the decomposition.

The above example particularly demonstrates the need for a "correction" of the sum "$1 + \rho_2\lambda_2 + \ldots + \rho_n\lambda_n$" by c in order to get a correct lower bound state in Theorem 2.4.

We next illustrate for a more advanced system that the lower bound mimics the behavior of the metastability for different decompositions of the state space. Consider the Smoluchowski dynamics

$$\gamma \mathrm{d}X = -\mathrm{grad}V(X)\mathrm{d}t + \sigma \mathrm{d}W_t$$

within a "perturbed" three well potential (see Fig. 1)

$$V(X) = 0.01\Big(X^6 - 30X^4 + 234X^2 + 14X + 100 + \quad (10)$$

$$30\sin(17X) + 26\cos(11X)\Big). \quad (11)$$

for given parameters $\gamma = 2$ and $\sigma^2 = 2\gamma/\beta$ with inverse temperature β. For a fixed observation time span $\tau = 1$ we discretize the transfer operator P_τ (for details or the discretization, see [27, 19]). For the comparison, we decompose the state space $\mathcal{X} = \mathbb{R}$ into the three subsets

$$A_1 = (-\infty, L], A_2 = (L, R], A_3 = (R, \infty)$$

for some parameters $L, R \in \mathbb{R}$ satisfying $L < R$. Figure 2 shows the calculated metastability $m(\mathcal{D})$ of the decomposition $\mathcal{D} = \{A_1, A_2, A_3\}$ and the lower bound according to Theorem 2.4 for two different values of inverse temperature. The case $\beta = 1$ mimics the situation of moderate metastability, while the case $\beta = 7$ corresponds to high metastability. As can be seen from Fig. 2, the lower bound is a good indicator for the actual metastability of the decomposition.

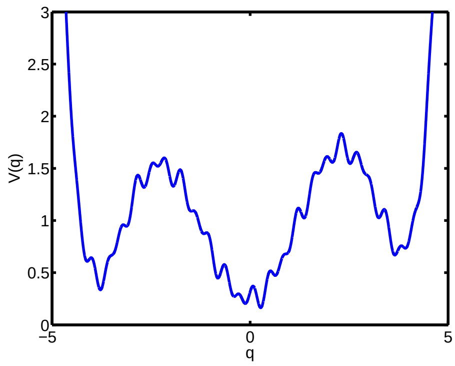

Figure 1: Graph of the perturbed three well potential V defined in (10).

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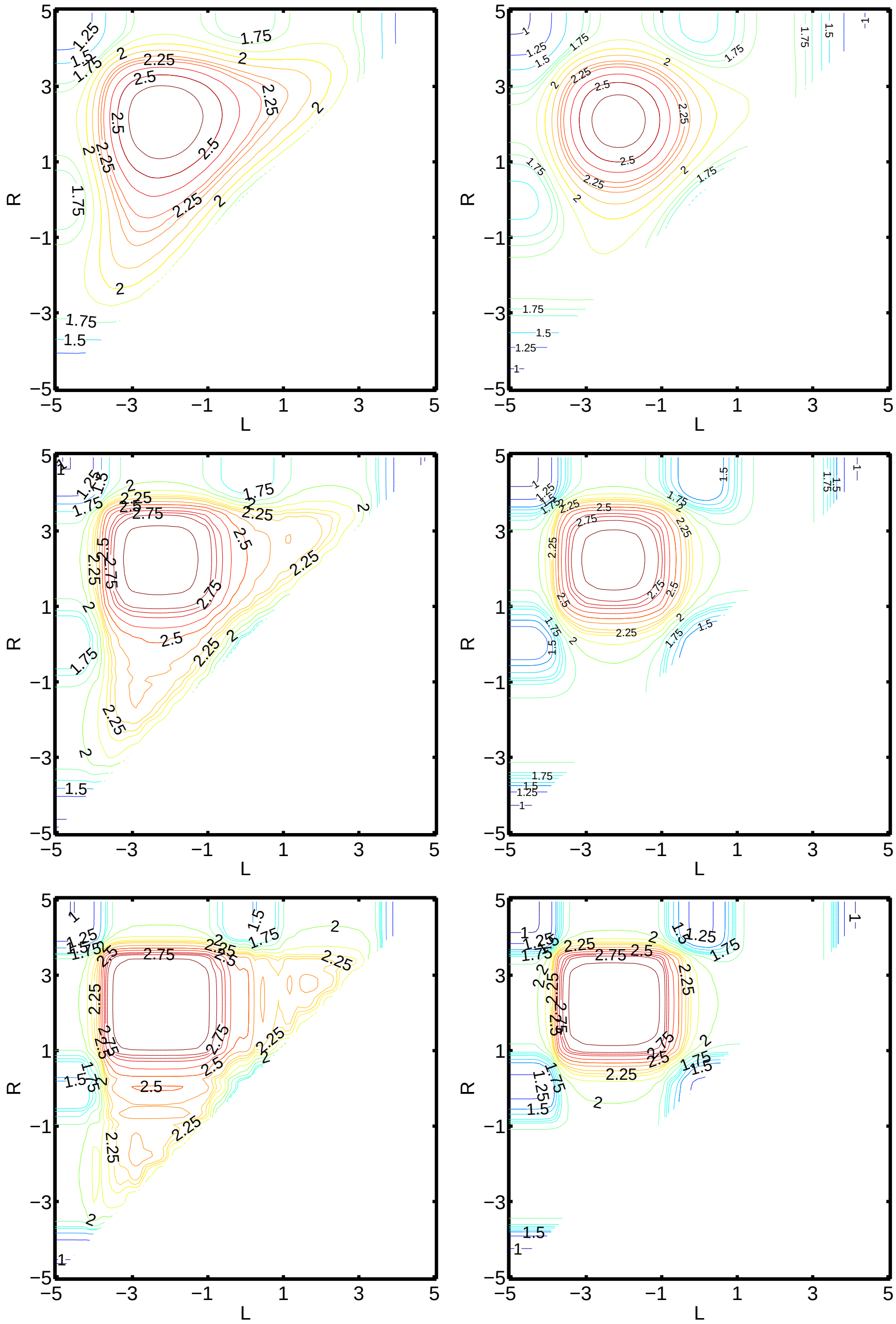

Figure 2: Metastability (left column) and lower bound (right column) corresponding to the perturbed three–well potential. From top to bottom increasing metastability due to increasing inverse temperature $\beta = 1$ (top), $\beta = 3$ (middle) and $\beta = 5$ (bottom).